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Re-runnable code is all you need

How to create reproducible and shareable computing environments

RSECon2024

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Re-Runnable Code is All You Need

1. **Introduction**
2. Deep Dive Devbox
3. Case Studies
4. Conclusion

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Introduction

Which terminology do we need in this talk?

Why does re-runnable code matter to us us?

How to select the right tooling?

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Introduction: Terminology

According to [1], research code should …

1. **Re-runnable**: be executable.
2. **Repeatable**: produce the same result more than once.
3. **Reproducible**: allow an investigator to reobtain the published results.
4. **Reuseable**: be easy to use, understand and modify.
5. **Replicable**: act as as an available reference for any ambiguity in the algorithmic descriptions of the article.

[1] Benureau, F. C., & Rougier, N. P. (2018). Re-run, repeat, reproduce, reuse, replicate: transforming code into scientific contributions. Frontiers in neuroinformatics, 11, 69.

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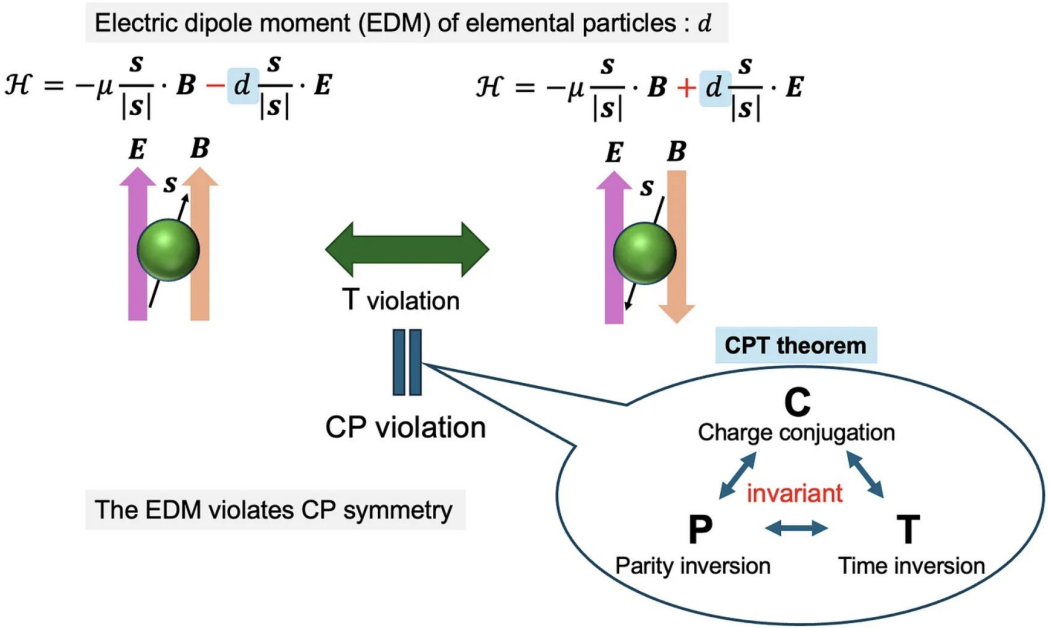
三の丸尚蔵館 大手門

Experiment: Matter-antimatter asymmetry in the universe



In case an Electric Dipole Moment (EDM) of elemental particles is found, then it violates the T symmetry (time) of the system. According to the CPT theorem, this would imply that the CP symmetry (charge and parity) is violated too. CP symmetry breaking is one of the candidate theories for explaining why there is a matter-antimatter asymmetry in the universe [2].

[2] A. D. Sakharov (1967). Violation of CP Invariance, C Asymmetry and Baryon Asymmetry of Universe, Journal of Experiment and Theoretical Physics Letters 5, 24-27.

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DT-01 CE 0598

Experiment: What happens when our code is not re-runnable

Symptoms:
- Automation becomes hard
- Collaboration is challenging

Possible root causes:
- Crucial steps are not defined in code
- Code is not designed to be shareable
- Environment variables are not managed well

[3] Blog post https://engineersforscience.substack.com/p/utokyo-case-study

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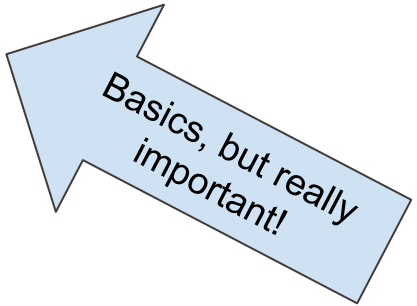
Experiment: The solution is often much simpler than we think ...

Solution:

- Define all steps in code
- Use proper package management
- Manage environment variables with configs

Take away:

- When we invest in the basics, they will help us everyday
- We use tooling to solve a problem, not because it is cool



[3] Blog post https://engineersforscience.substack.com/p/utokyo-case-study

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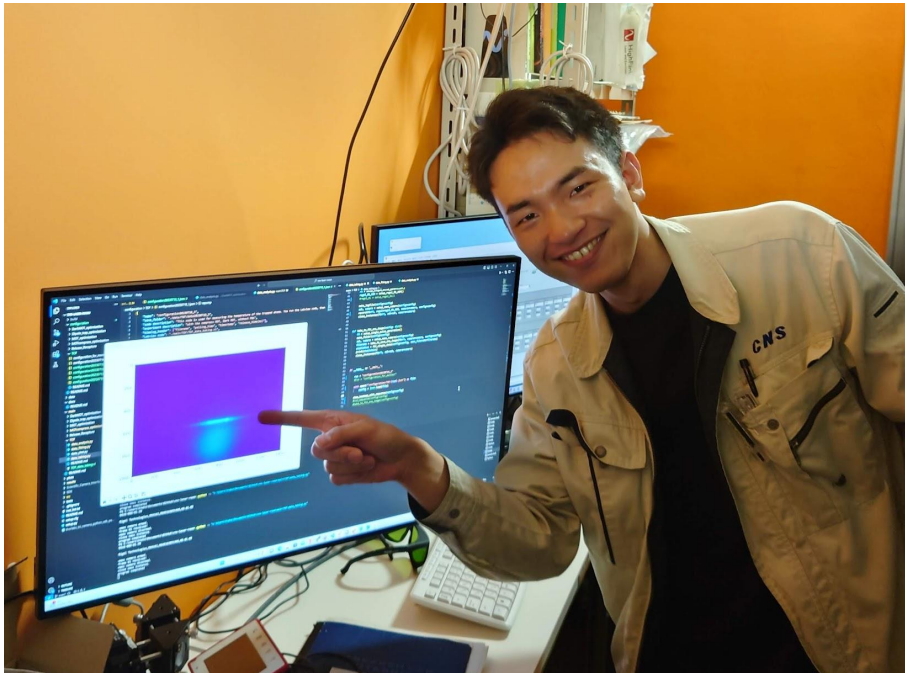
Experiment: … and makes the experiment successful!



July 2023: Nagase-san with the first atoms he captured with his Optical Dipole Trap

[3] Blog post https://engineersforscience.substack.com/p/utokyo-case-study

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Introduction: Terminology

1. **Version control**: Track changes and collaborate on code (Git).
2. **Package management**: Install and manage software libraries (pip).
3. **Environment management**: Ensure consistent software environments (devbox).
4. **Containerization**: Isolate software and dependencies (Docker).
5. **Workflow automation**: Automate repetitive tasks (GitHub Actions).
6. **Configuration management**: Maintain consistent software settings (Ansible).
7. **Infrastructure as Code (IaC)**: Code-based infrastructure setup. (Terraform).

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Introduction: Evaluating tools

Key factors for selecting an environment management tool:

- **Ease of Use**: Simple setup, intuitive commands, and minimal learning curve.
- **Integration with Version Control**: Seamless syncing with tools like Git.
- **Cross-Platform Compatibility**: Consistent behavior across macOS, Windows (WSL), and Linux.
- **Dependency Compatibility**: Supports diverse libraries and tools without conflicts.
- **Offline Usability**: Fully functional without internet access.
- **Performance**: Efficient resource usage; scales with project complexity.
- **Cost Efficiency**: Low or manageable costs for setup and maintenance.

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Deep Dive Devbox

- Re-runnable environments types
- Devbox - what is it?
  - How does it work?
  - Comparison with docker workflow
- Simple use-case
  - Different version of Node.js
  - Commands
- Github actions
- Usage in docker

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		Binary	
		Same	Different
Problem Domain	Same	**Reproducible**	**Re-runnable**
	Different	**Useful**	**Generalisable**

Copied and adapted from Richard Fitz John's talk on Tuesday

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What do you use for re-runnable environments?

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Some Re-runnable Environment Types

Language-specific	Developer Machines (mostly using PATH)	Binaries for Users (Virtualizations, chroot, …)	High Performance Computing
• nvm • gvm • pip / pyenv • maven	• devbox / flox • mise • asdf • brew / chocolatey • apt / yum / apk / rpm	• Docker • Flatpack • Snap	• spack • easybuild

Plus of course your personal favorite which is not on the list :)

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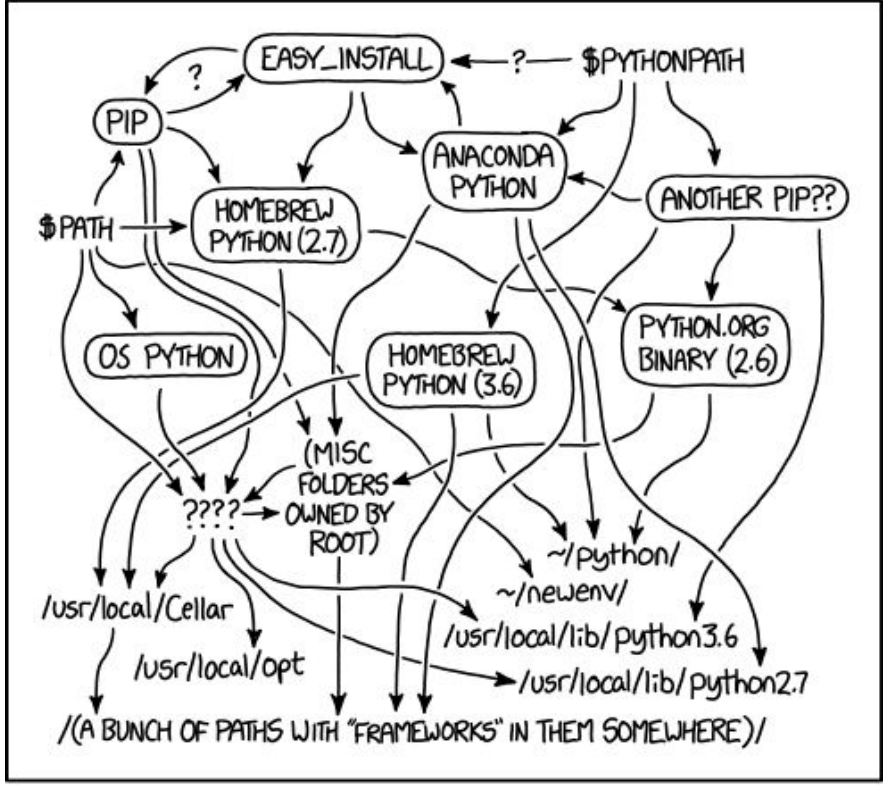

MY PYTHON ENVIRONMENT HAS BECOME SO DEGRADED
THAT MY LAPTOP HAS BEEN DECLARED A SUPERFUND SITE.

The Python environmental protection agency wants to seal it in a cement chamber, with pictorial messages to future civilizations warning them about the danger of using sudo to install random Python packages. - https://xkcd.com/1987/

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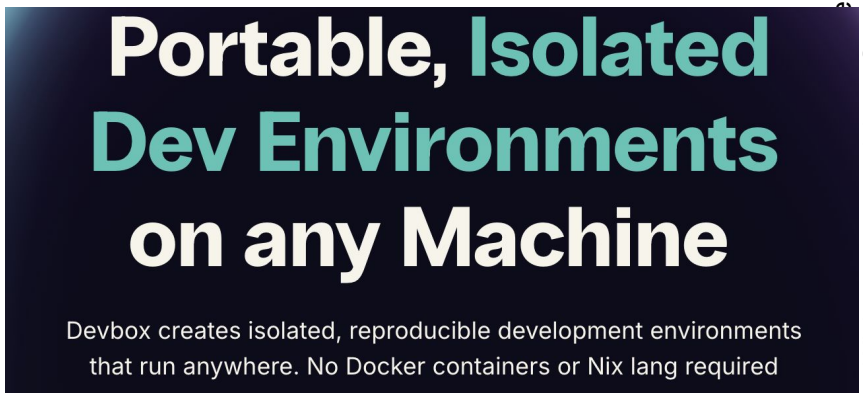
Devbox - TLDR;



Portable: runs on your laptop, github workflows, your customers' laptop, …

Isolated Dev Environment: use *that* version of node, golang, rust, java, etc. - isolation per shell

On any Machine: works on Linux, Mac, Windows WSL

Many many packages: over 400,000 versions of 80,000 packages powered by Nix

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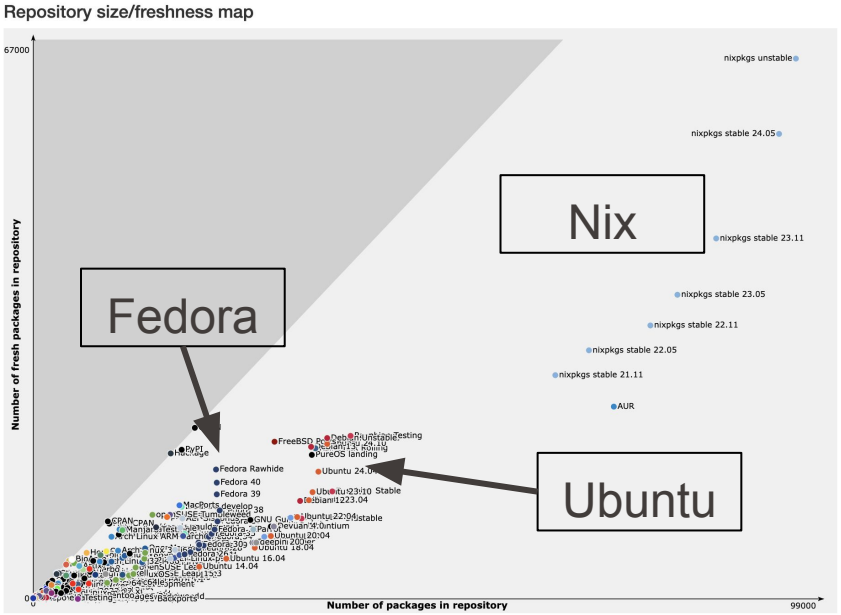
How does it work?

- Uses packages from Nix
  - Name it, nix got it
  - Installation is per-directory
- Versions are stored in *devbox.json* and *devbox.lock*
- Run your project in the `devbox shell` Environment
- Devbox sets PATH variable to those versions
  - Can be automated using `direnv`



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Simple Use-Case 1/2

Project with nodejs version 20, another with version 22

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How do you separate node versions for development?

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Simple Use-Case 1/2

Project with nodejs version 20, another with version 22

- Create directory and initialize devbox
  ```
  $ mkdir clash20 && cd clash20 && devbox init
  ```
  This creates an example *devbox.json*
- Install some packages
  ```
  $ devbox add nodejs@20 vim git
  ```
  Devbox either uses the local cache at /nix, or downloads the packages.
- Start using this environment
  ```
  $ devbox shell --pure # Don't include system cmds
  $ node --version
  v20.15.1 # At the time of this writing
  ```


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Simple Use-Case 2/2

Other project with nodejs version 22

- Create directory and initialize devbox

```
$ mkdir clash22 && cd clash22 && devbox init
$ devbox add nodejs@22 vim git
$ devbox shell --pure
$ node --version
v22.5.1
```

- Check nodejs version of other project

```
$ exit
$ cd ../clash20
$ devbox run -- node --version
v20.15.1
```


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devbox.json

```
{
  "$schema":
"https://raw.githubusercontent.com/.../devbox.schema.json",
  "packages": [
    "nodejs@22",
    "git@latest",
    "vim@latest"
  ],
  "shell": {
    "init_hook": [
      "npm ci"
    ],
    "scripts": {
      "test": [
        "npm test"
      ] } } }
```

It's a JSON-LD!

Packages and versions

Startup commands

Allows for simple scripting

To run it:

```
devbox run test
```

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Commands / Scripting

Similar to a very simple Makefile

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Did you ever write a Makefile from scratch?

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Commands / Scripting

Similar to a very simple Makefile:

- Environment variables for
  - Directory colors for *ls* with dark background
  - Run commands installed with *npm ci*
- Initialization when starting:
  - npm packages *npm ci*
  - make an alias for *ls*
- Three commands:
  - test - runs the tests with *npm test*
  - serve - serves the project with *ng serve*
  - build - builds the project with *ng build*

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devbox.json

```
"env": {
  "LS_COLORS": "di=33",
  "PATH": "$PATH:$PWD/node_modules/.bin"
},
"shell": {
  "init_hook": [
    "alias ls='ls --color'",
    "npm ci"
  ],
```

```
"scripts": {
  "test": [
    "npm test"
  ],
  "serve": [
    "ng serve"
  ],
  "build": [
    "ng build"
  ],
}
```


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Running commands

Now you can do a

`devbox run (test|serve|build)`

on any machine with devbox installed!

Or use

`devbox shell [--pure]`

to continue development.

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Github Actions

```yaml
name: Testing with devbox

on: push

jobs:
  test:
    runs-on: ubuntu-latest
    steps:
      - uses: actions/checkout@v3

      - name: Install devbox
        uses: jetify-com/devbox-install-action@v0.9.0

      - name: Run tests
        run: devbox run test
```


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And more

Create Dockerfile:

- `devbox build dockerfile`

Manage services:

- similar to docker-compose.yaml

Some paying options:

- Run in the cloud
  - devbox.sh/github.com/ineiti/fledger
- Run devcontainers

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Do you use a full CI/CD pipeline?
(Testing - Package publishing - Deploying)

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Case study - github.com/ineiti/fledger

Using devbox to:

- Easier onboarding of students
  - Install the rust toolchain
  - Include the wasm rust toolchain
- Only one source of tool versions
  - local installation vs. github-actions
- Github actions for CI/CD
  - Testing
  - Building docker files
    - Compiling in github action to use github cache for rust
  - Updating live servers (unchanged)

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Fledger - devbox.json rustup installation

```
{
  "packages": { "rustup": "latest", "trunk": "latest",
"wasm-pack": "latest" },
  "shell": {
    "init_hook": [
      "if [ ! -d $RUSTUP_HOME/toolchains/stable* ]; then
rustup default stable; fi",
      "if [ ! -d
$RUSTUP_HOME/toolchains/stable*/lib/rustlib/wasm32-unknown-u
nknown ]; then rustup target add wasm32-unknown-unknown;
fi",
    ],
    }
  }
```


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Fledger - single source of versions

Same version **locally**, in **github actions**, and in **Dockerfiles**:

```
-     - name: Install trunk
-       run: which trunk || cargo install --locked trunk
-
-     - uses: jetli/wasm-pack-action@v0.3.0
+     - name: Install devbox
+       uses: jetify-com/devbox-install-action@v0.11.0
        with:
```


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Fledger - github workflow

Replace direct calls with

`devbox run --`

so they use devbox

Profit!

```
      - name: Run cargo_build
-       shell: bash
-       run: |
-         make cargo_build
+       run: devbox run -- make cargo_build
```

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Fledger - Rust Linking Devbox Glibc

Problem:

```
$ file flsignal
...ELF 64-bit...interpreter
/nix/store/kz7xglxzhad64v667wwpn8vrxhjwcbna-glibc-2.39-52
/lib/ld-linux-x86-64.so.1
```

So it doesn't run in a minimal docker image.

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Fledger - Building Dockerfiles

```
FROM debian:bookworm-slim

RUN apt update && apt install patchelf

COPY target-common/release/flsignal flsignal
RUN patchelf --set-interpreter /usr/lib64/ld-linux-x86-64.so.2 flsignal

FROM debian:bookworm-slim
WORKDIR /fledger
COPY --from=0 flsignal /fledger/flsignal

ENTRYPOINT ["/fledger/flsignal", "-vv"]
```


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Fledger - rust/devbox shenanigans

```
{
  "packages": {...
    "darwin.apple_sdk.frameworks.SystemConfiguration": {
      "platforms": ["x86_64-darwin", "aarch64-darwin"]
    },
    "darwin.apple_sdk.frameworks.Security": {
      "platforms": ["x86_64-darwin", "aarch64-darwin"]
    },
  },
```


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Case Study - Tutorial Java Project [4]

- Easy installation
- Maven packages installation
  - per project - more space, but separation
  - global - faster installation, might collide

Some problems:

- How to run multi-line github actions with devbox?
  - Use devbox scripts

[4] Tutorial by Jaime Cardozo from the ETH Library

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Most difficult language re-runnable wise?

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The good, the bad, and the ugly

The Good

- Very simple configuration file
- Based on nix - huge collection of packages
- direnv can automate it even further

The Bad

- JSON configuration files - YAML would be nicer (comments, multi-line scripts)
- Some packages differ between platforms (e.g., psutils)
- Non-system compiler (openssl, rust-Security)
- No common shell history

The Ugly

- Non-root installation of devbox and nix is buggy

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Benefits of proper environment management

- **Time savings**: Streamlines onboarding, allowing new team members to get started faster.
  - Tip: A thorough onboarding document can save weeks of time.
- **Scientific impact**: Enhances the adoption of research findings and code by others.
  - Insight: This is based on our experience.
- **Productivity**: Reduces errors from version mismatches and environment issues.
- **Portability**: Makes research code more portable, enabling automation and cross-domain applications.

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Conclusion

- Environment management isn’t glamorous, but the productivity gains are!
- Devbox simplifies managing multiple environments by isolating them on a per-folder basis.
- For deployment, Devbox integrates seamlessly with Docker, eliminating the need to list endless dependencies in the Dockerfile.
- As RSEs, we have a responsibility to empower students and researchers with the right tools for effective and reproducible research.

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Special thanks go to Jaime Cardozo!

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Thank you!

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Backup slides

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Devbox vs. Dockerfile

Dockerfile

- Uses linux namespaces, with a linux VM on Windows / Mac
- *FROM* base package
  - Use package manager
  - Add packages
- Produces a docker image with all binaries
- Ready-to use application

Devbox

- Uses the system shell and packages compiled for the system
- Installs packages in sub-directories of */nix*
- Produces *devbox.json* and *devbox.lock* with references to installed packages
- Ready-to use development environment

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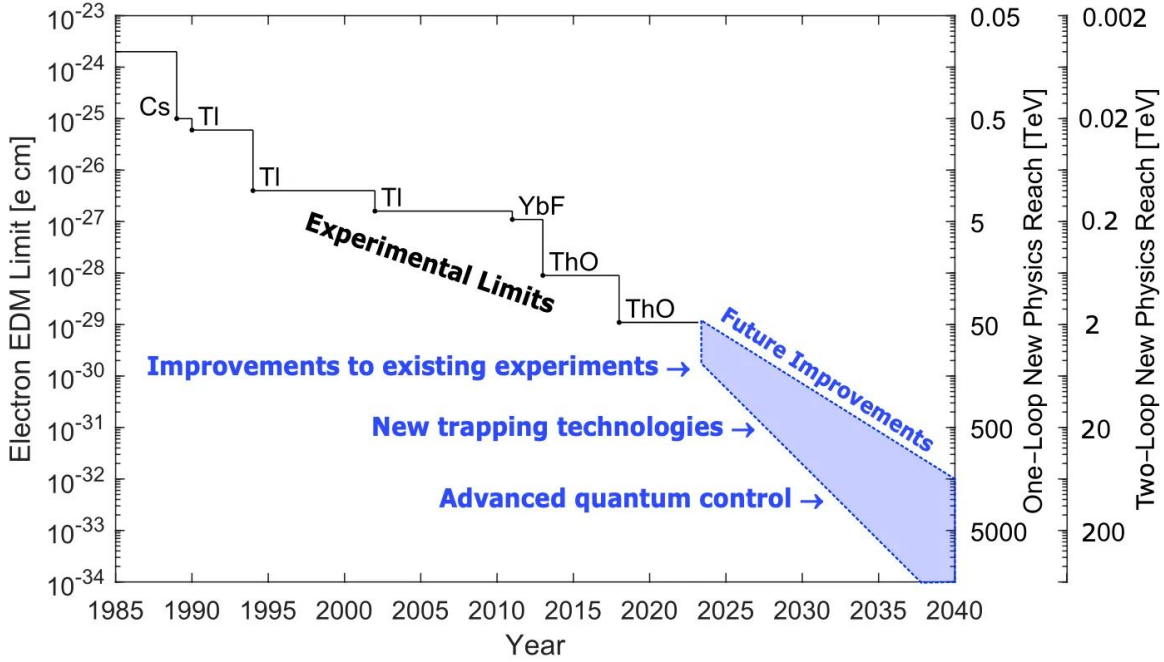
Experiment: Testing the Standard Model with cold atoms vs. colliders



Upper bound on the electron EDM over time, shown with the corresponding energy scale needed to observe new physics based on one-loop and two-loop effects. For comparison, colliders at CERN currently achieve a maximum collision energy of 13 TeV [2].

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[2] Chupp, T. E., Fierlinger, P., Ramsey-Musolf, M. J., & Singh, J. T. (2019). Electric dipole moments of atoms, molecules, nuclei, and particles. Reviews of Modern Physics, 91(1), 015001.

Case Studies

Real-life examples

- github.com/c4dt/rse.epfl.ch
  - Used by other members of EPFL
  - Hugo and rclone (plus some others)
  - Configuration for log-in is local and not in github…
- github.com/ineiti/fledger
  - Student project based on rust
  - Complete rust environment, including wasm
  - Docker-image generation

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rse.epfl.ch - goals

Our local RSE page:

- Using hugo
  - need the correct version
  - install the theme (git submodule)
  - let the user call hugo
- Pushing using rclone
  - Configuration of passwords is local
- Don't forget the README.md!

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rse.epfl.ch - hugo themes

```
{
  "packages": [... ],
  "shell": {
    "init_hook": [
      "if [ ! -f themes/anake/theme.toml ]; then git
submodule init && git submodule update; fi",
      "alias ls='ls --color'",
      "alias ll='ls -l --color'"
    ],
```


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rse.epfl.ch - command line arguments

```
{
  "packages": [... ],
  "shell": {
    "init_hook": [
      "if [ ! -f
themes/anake/theme.toml ]; then
git submodule init && git
submodule update; fi",
      "alias ls='ls --color'",
      "alias ll='ls -l
--color'"
    ],
```

```
"scripts": {
  "hugo": [
    "hugo $@"
  ],
  "server": [
    "hugo server -D"
  ],
  "update": [
    "git pull",
    "hugo",
    "rclone copy public/
ic-ftps:/rse.epfl.ch/"
  ]
```


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rse.epfl.ch - multi-line script

```
{
  "packages": [... ],
  "shell": {
    "init_hook": [
      "if [ ! -f
themes/anake/theme.toml ]; then
git submodule init && git
submodule update; fi",
      "alias ls='ls --color'",
      "alias ll='ls -l
--color'"
    ],
```

```
"scripts": {
  "hugo": [
    "hugo $@"
  ],
  "server": [
    "hugo server -D"
  ],
  "update": [
    "git pull",
    "hugo",
    "rclone copy public/
ic-ftps:/rse.epfl.ch/"
  ]
```


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